

First-exit-time probability density tails for a local height of a non-equilibrium Gaussian interface

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Abstract

We study the long-time behavior of the probability density Q_t of the first exit time from a bounded interval $[-L, L]$ for a stochastic non-Markovian process $h(t)$ describing fluctuations at a given point of a two-dimensional, infinite in both directions Gaussian interface. We show that Q_t decays when $t \rightarrow \infty$ as a power-law $t^{-1-\alpha}$, where α is non-universal and proportional to the ratio of the thermal energy and the elastic energy of a fluctuation of size L . The fact that α appears to be dependent on L , which is rather unusual, implies that the number of existing moments of Q_t depends on the size of the window $[-L, L]$. A moment of an arbitrary order n , as a function of L , exists for sufficiently small L , diverges when L approaches a certain threshold value L_n , and does not exist for $L > L_n$. For $L > L_1$, the probability density Q_t is normalizable but does not have moments.

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Non-equilibrium surface growth and dynamics of interfaces belong to an important multidisciplinary branch of non-equilibrium statistical mechanics, which received much interest within several last decades due to its numerous practical applications. To name just a few, we mention such diverse fields as crystal growth, molecular beam epitaxy, fluctuating steps of metal surfaces, evolution of liquid-liquid or liquid-vapor interfaces, and growing bacterial colonies [1, 2, 3]. A number of discrete atomistic models [1, 2, 3, 4] and stochastic evolution equations [5, 6, 7, 8, 9] has been proposed, revealing a generic scale invariance as manifest in the power law behavior of the interface width and correlation functions of the interface height. Much effort has been also expended in understanding universal aspects of different theoretical models and naturally occurring processes [1, 2, 3].

While earlier works have focused mainly on scaling behavior, more recent effort has been concentrated on evaluation of the distribution functions of characteristic properties of equilibrium or non-equilibrium interfaces. For different models of interfaces several probability distribution functions have been determined, including, e.g., the distribution of the width of heights in the steady state [10], maximal height distribution in one [11] and two-dimensions [12], distribution of spatially averaged height [13] or of the height at any fixed point in space [14], and the density of local maxima or minima of heights [15]. Last but not least, statistics of persistence, i.e., the probability that the interface height at a given point remains persistently above (or below) its initial value during some time interval, has been studied [16, 17].

In this paper we address a basic extreme value problem for a non-Markovian stochastic process $h(t)$, where $h(t)$ is a height (measured relative to the averaged value) at a fixed point of a non-equilibrium two-dimensional, infinite in both directions Gaussian interface, separating two phases in $d = 3$. Using the approach of Refs.[18], we determine the long-time asymptotical behavior of the "survival" probability P_t that $h(t)$ does not leave within the time interval $(0, t)$ a bounded interval $[-L, L]$, and correspondingly, define the tail of the probability density Q_t of the first-exit-time t from $[-L, L]$, $Q_t \sim -dP_t/dt$. We show that in a striking contrast to the one-dimensional case, where $P_t \sim \exp(-t^{1/2}/L^2)$ [18, 19], and hence, Q_t has all moments, for a two-dimensional Gaussian interface the probability Q_t is characterized by a power-law tail of the form

$$Q(t) \sim \frac{1}{t^{1+\alpha}}, \quad t \gg \kappa^{-1} \exp\left(\frac{\kappa L^2}{T}\right), \quad (1)$$

T being the temperature (measured in the units of the Boltzmann constant k_B) and κ - the interfacial tension. The exponent α in Eq.(1) is non-universal:

$$\alpha = C \frac{T}{2\kappa L^2}, \quad (2)$$

where C is a constant, such that $\pi/16 \leq C \leq \pi/8$. The exponent α is thus proportional to the ratio of the thermal energy and the elastic energy of a fluctuation of size L . As a consequence of the L -dependence of α , not all moments of Q_t exist and, what is rather unusual, the very number of existing moments of Q_t depends on the size of the window $[-L, L]$.

Consider a two-dimensional interface whose local heights $h_{n,m}(t)$, measured relative to the averaged value, obey an infinite set of Langevin equations [20]:

$$\xi \frac{dh_{n,m}(t)}{dt} = \kappa \left(h_{n+1,m}(t) + h_{n-1,m}(t) + h_{n,m+1}(t) + h_{n,m-1}(t) - 4h_{n,m}(t) \right) + \zeta_t^{(n,m)}, \quad (3)$$

where $-\infty < n, m < \infty$ and $\zeta_t^{(n,m)}$ are independent Gaussian white-noise processes:

$$\overline{\zeta_t^{(n,m)}} = 0, \quad \overline{\zeta_t^{(n,m)} \zeta_{t'}^{(n',m')}} = 2\xi T \delta_{n,n'} \delta_{m,m'} \delta(t - t'). \quad (4)$$

In Eqs.(3) and (4), ξ is the friction coefficient, the bar denotes averaging over thermal histories, $\delta_{n,n'}$ is the Kronecker-delta symbol and $\delta(t)$ - the delta-function. In what follows we set, for simplicity, $\xi = 1$, such that the appropriate dimensionless "time" variable will be κt . Dependence on ξ can be restored in our final results by a mere replacement $T \rightarrow T/\xi$ and $\kappa \rightarrow \kappa/\xi$.

Note that Eqs.(3) describe, in particular, the time evolution of a spatially discretized Edwards-Wilkinson interface [5], as well as model A Langevin dynamics [20] of the Weeks columnar model [21] or of a coarse-grained interface in a three-dimensional Ising model above the roughening temperature [22].

We suppose that initially the interface is flat and $h_{n,m}(t = 0) = 0$ for all n and m . Applying to Eqs.(3) a discrete Fourier transformation, solving the resulting equation and inverting the solution, we find that, for a given thermal history, the local height at the origin $h(t) = h_{0,0}(t)$ is defined as a portfolio of an infinite number of weighted independent Gaussian processes:

$$h(t) = \int_0^t d\tau e^{-4\kappa\tau} \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} I_n(2\kappa\tau) I_m(2\kappa\tau) \zeta_{t-\tau}^{(n,m)}, \quad (5)$$

where $I_n(2\kappa\tau)$ is the modified Bessel function of order n . From Eq.(5) one finds that at sufficiently long times [22]:

$$\overline{h^2(t)} \sim \frac{T}{4\pi\kappa} \ln(\kappa t). \quad (6)$$

Our aim is now to define, for a non-Markovian process $h(t)$ in Eq.(5), the probability P_t that $h(t)$ has not ever crossed the boundaries of the interval $[-L, L]$ within the time interval $(0, t)$ given the initial condition $h(t=0) = 0$, i.e., $P_t = \text{Prob}(\max|h(t)| < L | h(0) = 0)$, where $\max|h(t)|$ is the largest absolute value achieved by $h(t)$ within the time interval $(0, t)$. Once P_t is determined, we will get an access to the behavior of another important probability - the first-exit-time probability density $Q_t = \text{Prob}(t' > t | h(0) = 0)$, where $t' = \min\{\tau | h(\tau) = \pm L\}$ is the time when $h(t)$ first hits either of the boundaries; hence, Q_t is defined as

$$Q_t dt \equiv -\frac{dP_t}{dt} dt = \text{Prob}(t < t' \leq t + dt | h(0) = 0). \quad (7)$$

Focusing on the large- t asymptotical behavior, we note that it is not really important how we define $\zeta_t^{(n,m)}$ - as continuous in time functions or as discrete processes, provided that we keep all essential features of noise. We thus divide, at fixed t , the interval $(0, t)$ into N small subintervals Δ , (such that $\Delta N \equiv t$), and assume that

$$\zeta_\tau^{(n,m)} = \left(\frac{2T}{\Delta}\right)^{1/2} S_{[\tau/\Delta]}^{(n,m)}, \quad (8)$$

where $[x]$ denotes the floor function. In other words, we assume that $\zeta_\tau^{(n,m)}$ is constant and equal to $\sqrt{2T/\Delta} S_k^{(n,m)}$ within the k -th subinterval, $k = 0, 1, \dots, N-1$, where $\{S_k^{(n,m)}\}$ is an infinite set of independent identically distributed random variables with normal distribution $N[0, 1]$.

Then, $h(t)$ can be expressed as a weighted sum of an infinite number of independent discrete noise processes:

$$h(N) = \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \sum_{l=1}^N \sigma_l^{(n,m)} S_{N-l}^{(n,m)}, \quad (9)$$

with weights

$$\sigma_l^{(n,m)} = \left(\frac{T}{2\Delta\kappa^2}\right)^{1/2} \int_{2\kappa\Delta(l-1)}^{2\kappa\Delta l} du e^{-2u} I_n(u) I_m(u). \quad (10)$$

Squaring Eq.(9) and averaging the resulting expression with respect to the distribution of i.i.d. variables $\{S_k^{(n,m)}\}$, we get

$$\overline{h^2(N)} = \sum_{l=1}^N \tilde{\sigma}_l^2, \quad (11)$$

which expression introduces an effective variance $\tilde{\sigma}_l^2$, defined as

$$\tilde{\sigma}_l^2 = \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \left(\sigma_l^{(n,m)} \right)^2 = \frac{T}{2\Delta\kappa^2} \int_{2\kappa\Delta(l-1)}^{2\kappa\Delta l} du_1 \int_{2\kappa\Delta(l-1)}^{2\kappa\Delta l} du_2 f(u_1, u_2), \quad (12)$$

where

$$f(u_1, u_2) = e^{-2u_1 - 2u_2} I_0^2(u_1 + u_2). \quad (13)$$

Noticing that $\exp(-2x)I_0^2(x)$ is a monotonically decreasing function of x , one finds that $\tilde{\sigma}_l^2$ is bounded by two monotonically decreasing functions of l :

$$\exp(-8\kappa\Delta l) I_0^2(4\kappa\Delta l) \leq \frac{\tilde{\sigma}_l^2}{2\Delta T} \leq \exp(-8\kappa\Delta(l-1)) I_0^2(4\kappa\Delta(l-1)). \quad (14)$$

When $l \gg 1$, these bounds become very sharp and hence, with a good accuracy,

$$\tilde{\sigma}_l^2 \approx 2\Delta T \exp(-8\kappa\Delta l) I_0^2(4\kappa\Delta l). \quad (15)$$

Substituting Eq.(15) into Eq.(11), we recover the result in Eq.(6).

Define now the following event: An N -step discrete-time trajectory $h(N)$, Eq.(9), commencing at the origin, does not leave the interval $[-L, L]$, or in other words, the maximal absolute value, $\max|h(N)|$, which process $h(N)$ achieves for a given realization of noise, is less than L . Probability of such an event we denote as $P_N = \text{Prob}(\max|h(N)| < L)$.

Now, condition $\max|h(N)| < L$ implies that the absolute value of any ascending partial sum

$$h_k(N) = \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \sum_{l=N-k+1}^N \sigma_l^{(n,m)} S_{N-l}^{(n,m)}, \quad (16)$$

which define the values of the local height $h(N)$ at consecutive discrete "time" moments k , $k = 1, 2, \dots, N$, is bounded from above by L .

We prefer, however, to deal with the *descending* partial sums:

$$h'_k(N) = \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \sum_{l=1}^k \sigma_l^{(n,m)} S_{N-l}^{(n,m)}, \quad (17)$$

which define the trajectory $h_k(N)$ evolving in the inverse time $N - k$ and shifted by a constant (realization-dependent) value $h_N(N)$. Clearly, $P_N = \text{Prob}(\max|h(N)| < L) = \text{Prob}(\max|h'(N)| < L)$.

Let $I(\max|h'(t)| < L)$ be the indicator function:

$$I(\max|h'(N)| < L) = \begin{cases} 1, & \max|h'(N)| < L, \\ 0, & \max|h'(N)| > L. \end{cases} \quad (18)$$

and $R_L(x)$ - a rectangular function, such that:

$$R_L(x) = \int_{-\infty}^{\infty} \frac{dy \sin(Ly)}{\pi y} e^{iyx} = \begin{cases} 1, & |x| < L, \\ 1/2, & x = \pm L, \\ 0, & |x| > L. \end{cases} \quad (19)$$

Then, using the definition of the descending partial sums in Eq.(17) and Eq.(19), we write down Eq.(18) as the following N -fold integral:

$$I(\max |h'(N)| < L) = \prod_{k=1}^N I(|h'_k(N)| < L) = \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} \prod_{k=1}^N \frac{dy_k \sin(Ly_k)}{\pi y_k} e^{i y_k h'_k(N)}. \quad (20)$$

Averaging the indicator function in Eq.(20) with respect to the distribution of i.i.d. random variables $\{S_k^{(n,m)}\}$, and changing integration variables (see Refs.[18] for more details), we find eventually the following exact representation of P_N :

$$P_N = \int_{-L}^L \dots \int_{-L}^L \prod_{k=1}^N \frac{dh_k}{\sqrt{2\pi}\tilde{\sigma}_k} \exp \left[-\frac{(h_k - h_{k-1})^2}{2\tilde{\sigma}_k^2} \right], \quad (21)$$

where h_0 is fixed, $h_0 \equiv 0$. Once P_N is known, the desired survival probability P_t can be obtained as an appropriate limit: $P_t = \lim_{\Delta \rightarrow 0, N \rightarrow \infty} P_N$, with $\Delta N = t$ kept fixed.

The N -fold integral in Eq.(21) can not be, of course, evaluated exactly and one has to resort to controllable approximations. Here, using the approach of Refs.[18], we construct rigorous lower and upper bounds on P_N in Eq.(21), taking an advantage of the following property of P_N in Eq.(21) [18]:

$P_N = P_N(\tilde{\sigma}_1, \tilde{\sigma}_2, \tilde{\sigma}_3, \dots, \tilde{\sigma}_N)$ is a monotonically decreasing function of any variable $\tilde{\sigma}_k$.

This signifies that replacing any or all $\tilde{\sigma}_k$ by $\Sigma(k)$, such that $\tilde{\sigma}_k \leq \Sigma(k)$, we will decrease the right-hand-side of Eq.(21) and arrive at the *lower* bound on P_N ; if, on contrary, we will replace one or all $\tilde{\sigma}_k$ by $\tilde{\Sigma}(k)$, such that $\tilde{\sigma}_k \geq \tilde{\Sigma}(k)$, we will *increase* the right-hand-side of Eq.(21) and obtain an *upper* bound on P_N .

We start with a lower bound on P_N . As we have already noticed, $\exp(-2x)I_0^2(x)$ in Eq.(12) is a monotonically decreasing function of x . Consequently, setting in the integrand $u_2 \equiv 0$, and integrating over du_2 , we have

$$\tilde{\sigma}_k^2 \leq \Sigma(k)^2 = \frac{T}{\kappa} \int_{2\kappa\Delta(k-1)}^{2\kappa\Delta k} du e^{-2u} I_0^2(u) = t_k^{(upp)} - t_{k-1}^{(upp)}, \quad (22)$$

where

$$t_k^{(upp)} \equiv \frac{T}{\kappa} \int_0^{2\kappa\Delta k} du e^{-2u} I_0^2(u). \quad (23)$$

Therefore, P_N in Eq.(21) is bounded from *below* by

$$P_N \geq \int_{-L}^L \cdots \int_{-L}^L \prod_{k=1}^N \frac{dh_k}{\sqrt{2\pi (t_k^{(upp)} - t_{k-1}^{(upp)})}} \exp \left[-\frac{(h_k - h_{k-1})^2}{2 (t_k^{(upp)} - t_{k-1}^{(upp)})} \right], \quad (24)$$

where h_0 is fixed, $h_0 \equiv 0$.

One notices now that the expression on the right-hand-side of Eq.(24) describes the probability that an N -step trajectory of a Brownian motion evolving in "time" $t_k^{(upp)}$ does not leave an interval $[-L, L]$, which yields, in the leading order,

$$P_N \geq \exp \left(-\frac{\pi^2}{8L^2} t_N^{(upp)} \right) = \exp \left(-\frac{\pi^2 T}{8\kappa L^2} \int_0^{2\kappa\Delta N} du \exp(-2u) I_0^2(u) \right). \quad (25)$$

Defining the asymptotical large- N behavior of the integral in the exponential in Eq.(25) and turning to the limit $\Delta \rightarrow 0$, $N \rightarrow \infty$ with $\Delta N = t$ kept fixed, we arrive at the following lower bound on P_t :

$$\frac{\ln(P_t)}{\ln(\kappa t)} \geq -\frac{\pi}{8} \frac{T}{2\kappa L^2}, \quad \kappa t \gg \exp(\kappa L^2/T). \quad (26)$$

Consider next an *upper* bound on P_N , Eq.(21). Using the inequality in Eq.(14) and an evident inequality: $\exp(-2x) I_0^2(x) \geq 1/(2\pi x + 1)$, which holds for any $x \geq 0$, we have

$$\tilde{\sigma}_k^2 \geq 2\Delta T \exp(-8\kappa\Delta k) I_0^2(4\kappa\Delta k) \geq \frac{2\Delta T}{8\pi\kappa\Delta k + 1} \geq \tilde{\Sigma}(k)^2 = t_k^{(low)} - t_{k-1}^{(low)}, \quad (27)$$

whith

$$t_k^{(low)} = \frac{T}{4\pi\kappa} \ln(8\pi\kappa\Delta(k+1) + 1). \quad (28)$$

Hence, in virtue of Eq.(27), P_N in Eq.(21) is bounded from *above* by

$$P_N \leq \int_{-L}^L \cdots \int_{-L}^L \prod_{k=1}^N \frac{dh_k}{\sqrt{2\pi (t_k^{(low)} - t_{k-1}^{(low)})}} \exp \left[-\frac{(h_k - h_{k-1})^2}{2 (t_k^{(low)} - t_{k-1}^{(low)})} \right], \quad (29)$$

where h_0 is fixed, $h_0 \equiv 0$.

One recognizes now that the rhs of Eq.(29) is the probability that an N -step trajectory of a Brownian motion evolving in "time" $t_k^{(low)}$ does not leave an interval $[-L, L]$. Hence, the following *upper* bound on P_N is valid:

$$P_N \leq \exp \left(-\frac{\pi^2}{8L^2} t_N^{(low)} \right) \sim \exp \left(-\frac{\pi T}{16\kappa L^2} \ln(\kappa\Delta N) \right), \quad (30)$$

which yields the following upper bound on P_t :

$$\frac{\ln(P_t)}{\ln(\kappa t)} \leq -\frac{\pi}{16} \frac{T}{2\kappa L^2}, \quad \kappa t \gg \exp(\kappa L^2/T). \quad (31)$$

Since P_t is, evidently, a monotonically decreasing function of time, we infer that the large- t asymptotical behavior of P_t is described by a power-law of the form $P_t \sim (\kappa t)^{-\alpha}$, where $\alpha = CT/2\kappa L^2$ and C is a constant, such that $\pi/16 \leq C \leq \pi/8$. Consequently, the long-time tail of the first-exit-time probability density Q_t is a power-law, $Q_t \sim t^{-1-\alpha}$, Eq.(1).

In conclusion, we have shown that the probability density Q_t of the first-exit-time t from a bounded interval $[-L, L]$ for a non-Markovian process $h(t)$ describing fluctuations at a given point of a two-dimensional, infinite in both directions Gaussian interface, is characterized by a power-law tail in Eq.(1). The exponent α is non-universal and proportional to the ratio of the thermal energy and the elastic energy of a fluctuation of size L , and thus depends on L . We note that a power-law behavior of P_t is not counterintuitive, and could, in principle, be expected from a heuristic estimate $P_t \sim \exp(-\overline{h^2(t)}/L^2)$ [23] combined with a logarithmic growth of the second moment of $h(t)$, Eq.(6). On the other hand, the dependence of α on L is a rather unusual fact which entails unusual behavior of the moments of Q_t ; namely, the number of existing moments of Q_t appears to be defined by the size of the window in which the stochastic process $h(t)$ is observed. More specifically, the number n of existing moments depends on the relation between L and a discrete set of characteristic lengths $L_n = (CT/2\kappa n)^{1/2}$; the condition that Q_t has exactly n moments is, in fact, equivalent to the requirement that L obeys the following double-sided inequality: $L_{n+1} < L < L_n$. In other words, a moment of an arbitrary order n , as a function of L , exists for sufficiently small L , diverges when L approaches L_n , and does not exist for $L > L_n$. For $L \geq L_1$, the probability density Q_t is normalizable but does not have moments. We note finally that an analogous behavior can be expected for the interfaces defined by noisy Mullins equation [6] in $d = 5$ or by general linear Langevin equations described in Refs.[8, 9] in $d = 3$.

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